

REANALYSIS OF MIPAS ESA V6 CH₄ AND N₂O

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ABSTRACT

This study describes reanalyses of MIPAS CH₄ and N₂O observations by the Belgian Assimilation System for Chemical Observations (BASCOE). Here, MIPAS ESA v6 at the optimized spectral resolution and from the nominal mode of observations have been assimilated. The study shows the added value of data assimilation in using the information of the averaging kernels as well as the information of the background error covariance matrix. This allows the system to regularize the vertical distribution of CH₄ and N₂O, which presents vertical oscillations in the MIPAS ESA observations. The reanalyses agree generally well with ACEFTS v3.5. Nevertheless, unrealistic time discontinuities that come from the assimilated data are found such that filtering/averaging of these reanalyses will be necessary.

1. INTRODUCTION

Carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O) are the three most important well-mixed greenhouse gases (WMGHG, Stocker et al., 2013). Their contributions in enhancing radiative forcing are, respectively, 1.82, 0.48 and 0.17 Wm⁻². After a decade of near stability, the increase of CH₄ concentration has been observed and the radiative forcing from CH₄ is now larger than all of the combined halocarbons. The concentration of N₂O is also increasing such that, due to the decrease of chlorofluorocarbons 12 (CFC-12), N₂O is now the third largest WMGHG contributor to radiative forcing.

Modelling the atmospheric radiative forcing requires a relatively accurate representation of these species. Moreover, several studies have acknowledged the impact of the stratospheric representation in numerical weather prediction and climate models (Monge-Sanz et al., 2013, and references therein). This is in particular the case for O₃, H₂O, CH₄ and CFCs. However, the computing time to resolve state-of-the-art chemical equation systems for the stratosphere is much too expensive for those models, that usually also account for troposphere, land-surface, sea-

ice and ocean processes (with different degree of complexity). For this reason, linearized chemical schemes have been developed, with much more attention to O₃. These linear schemes are usually based on a climatological representation of the gas of interest. As the complexity of climatologies (e.g. 2-dimensional vs. 3-dimensional) impacts on model results, the aim of this study is to provide reanalyses of CH₄ and N₂O from which 4-dimensional (i.e. depending on latitude, longitude, altitude and time) climatologies will be built.

This paper is organized as follows. Sect. 2 presents the assimilated data. The Belgian Assimilation System for Chemical Observations (BASCOE) and its setup is presented in Sect. 3. Sect. 4 presents the CH₄ and N₂O reanalyses, in particular its validation. Finally, Sect. 5 summarizes the results of this paper.

2. ASSIMILATED OBSERVATIONS

Assuming that we need a data records of several years with a relatively high spatial coverage, the only possible choice for the CH₄ assimilated data are the MIPAS observations. Several retrievals are available for MIPAS CH₄ and we have considered two of them: the ESA v6 and the IMK/IAA V5R. Both datasets have issues. IMK/IAA is known to be high biased in the equatorial (Eq) lower stratosphere (LS) and low biased in the polar vortex (Glatthor et al., 2005), as shown in Figure 1. On the other hand, the ESA retrieval is known to produce oscillated profiles in the EqLS (Payan et al., 2009). However, the use of averaging kernels provided in the MIPAS ESA data files reduces these oscillations in the BASCOE analyses (see Sect. 4), such that this dataset has been chosen for CH₄.

These two MIPAS retrievals have the same issues for N₂O. For the same reasons as for CH₄, ESA retrieval was chosen. In addition to MIPAS, other satellite observations are available for N₂O, from Aura MLS and Odin SMR. We do not consider Odin SMR. At the beginning of the work, the aim was to assimilate simultaneously MIPAS ESA and MLS data. The advantage of such strategy

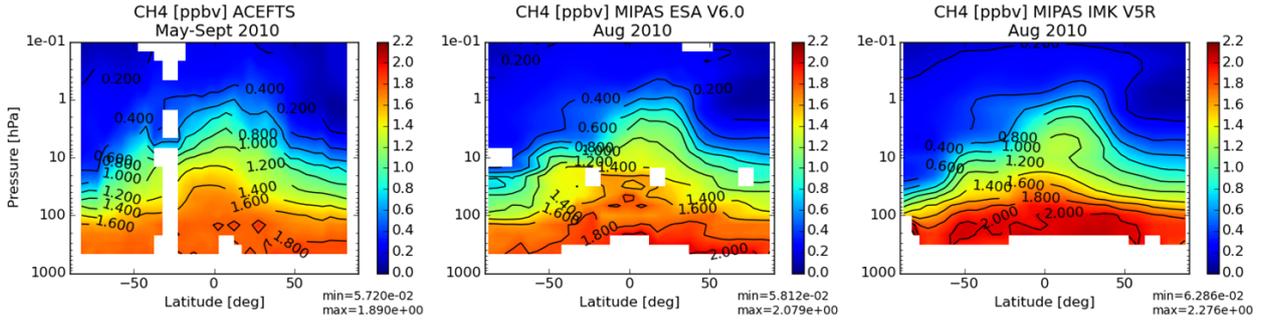


Figure 1. Zonal mean of CH_4 retrieved by ACEFTS v3.5 for May-September 2010 (left), MIPAS ESA v6 for August 2010 (center) and MIPAS IMK/IAA V5R for August 2010 (right).

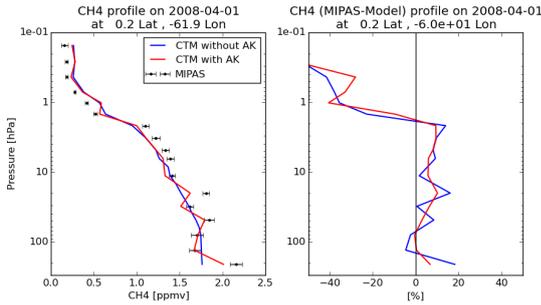


Figure 2. (Left) MIPAS CH_4 profile as compared to BASCOE interpolated at MIPAS using or not the averaging kernels in the interpolation. (Right) Differences between MIPAS and the two BASCOE profiles.

would have been the following. First, MLS operates almost continuously while MIPAS has several missing days of observations in particular in 2005 and 2006. MIPAS has also several switches between its mode of measurement (only the nominal mode is used in this study). The second advantage would have been to implement N_2O - CH_4 correlations in the background error covariance matrix. Because of the discontinuities in MIPAS operations, MLS N_2O data would have been useful to constrain CH_4 during time of missing MIPAS data. Assimilating N_2O from MIPAS and MLS would require to remove the biases between these two datasets, something we failed to achieve. It led us to choose the N_2O datasets to assimilate between MIPAS ESA and MLS. Above 10 hPa, the error bars of MLS v3.3 N_2O increase (41 % at 4.6 hPa, 100 % at 1 hPa, Livesey et al., 2011) and thus these observations provide only a small constraint to the assimilation scheme. For this reason, we decided to assimilate MIPAS ESA v6 N_2O observations which error bars remain lower than 20 % below 45 km (around 1 hPa, Raspollini et al., 2013).

Optimal resolution measurements from the MIPAS nominal mode have been assimilated, between January 2005 and April 2012. The observational error used in the assimilation system are given by the ESA retrieval with a minimum value of 5 %. A background quality check (Anderson and Järvinen, 1999) is operated on the each

individual profile point with a threshold value of 5: profiles that failed to fill the following condition are rejected: $(y - H(\mathbf{x}))^2 < 5(\sigma_y^2 + \sigma_x^2)$ where \mathbf{x} is the model state vector, y is the observation vector, H is the observation operator, σ_x is the background error standard deviation vector and σ_y is the observation standard deviation vector.

The averaging kernels of MIPAS have been used. In data assimilation, the averaging kernels allow one to remove the information of the a priori from the observations as follow:

$$\mathbf{x} = \mathbf{y}_0 + \tilde{\mathbf{A}} [\tilde{\mathbf{x}} - \tilde{\mathbf{y}}_0] \quad (1)$$

where \mathbf{x} is the model profile, \mathbf{y}_0 is the a priori profile used to retrieve the observed profile, \mathbf{A} is the averaging kernel matrix and “ \sim ” indicate that the vectors are on the model vertical grid (for matrices, only the rows is on the model vertical grid). With MIPAS ESA, the situation is different because the retrieval algorithm does not rely on any a priori profile. In that case, \mathbf{y}_0 must be replaced by \mathbf{y}_{k-1} where k is the number of iteration of the retrieval (Ridolfi et al., 2011). The MIPAS ESA data files do not provide \mathbf{y}_{k-1} . Since the convergence criteria of the retrieval are rather conservative, the MIPAS quality working group recommend to use \mathbf{y}_k in Eq. (1), in place of \mathbf{y}_0 .

Figure 2 illustrates the impact of the use of averaging kernels when comparing BASCOE model and MIPAS. The figure displays a CH_4 profile in the tropics which clearly shows oscillations below 10 hPa. Two BASCOE model profiles interpolated at MIPAS are also shown. One profile is interpolated without using the averaging kernels whereas the second profile is interpolated using the averaging kernels. The first BASCOE profile is relatively smooth, as expected, and the second BASCOE profile shows oscillations. Overall, the difference profile between MIPAS and BASCOE is much smoother when averaging kernels are used than when they are not used. In the end, the analysis increment becomes much smoother, and reliable, when the averaging kernels are used.

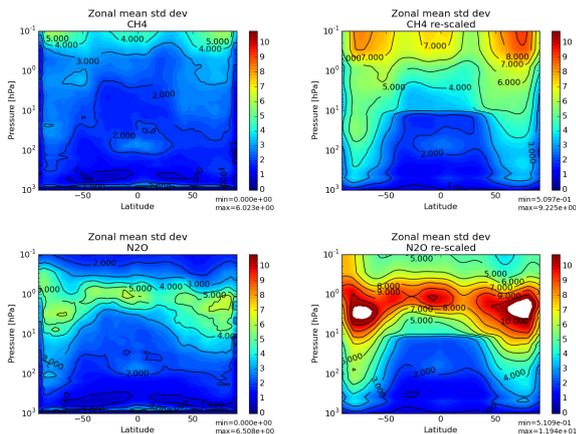


Figure 3. Zonal mean of the background error standard deviation [%] estimated by the ensemble method. From top left to bottom right: CH_4 , CH_4 scaled, N_2O and N_2O scaled.

3. THE BASCOE SYSTEM

This study is based on data assimilation experiments using the Belgian Assimilation System for Chemical Observations (BASCOE; Errera et al., 2008; Viscardy et al., 2010). This system is based on the 4D-Var method and a chemistry transport model (CTM) driven by ECMWF ERA-Interim reanalysis (Dee et al., 2011). The background error covariance matrix (\mathbf{B} matrix) is formulated on a spherical harmonic basis assuming homogeneous and isotropic correlations (Errera and Ménard, 2012). The \mathbf{B} matrix has been calibrated using an ensemble method (Fisher, 2003). The concept is the following. An ensemble of assimilation experiments are performed. For each members, the assimilated dataset and the model initial condition are made from a perturbation of, respectively, the real observations and a reference initial condition. Given the number of members and assimilation cycle, an ensemble of short terms forecast difference is constructed. Based on several assumptions (Bannister, 2008), it can be shown that this ensemble of short term forecast difference is a sample of the \mathbf{B} matrix such that its properties can be estimated. For the reanalysis discussed here, two members are used and the assimilation period is between March 2008 and 2009. Thus the \mathbf{B} matrix is calibrated for a year and the same setup is used for each year and season of the reanalysis.

Figure 3 shows the zonal mean of the background error standard deviation matrix for CH_4 and N_2O . Note that the ratio between the background error standard deviation matrix and the observational error standard deviation matrix will set the weight between of the background state and the observations in the final analysis. For CH_4 , the background standard deviation error is generally below or around 2% in the EqLS and increases to 2% at the poles and to 3% above 1 hPa. For N_2O , this error is around 2% in the EqLS and increases slightly near the poles (3% at South Pole) and also increases with altitude with a max-

imum of 5% at 1 hPa. Since MIPAS data are accurate above 10 hPa and at the poles, and since the model is known to overestimate CH_4 and N_2O in the polar vortex, the background standard deviation error has been doubled in those regions (see Figure 3) in order to increase the weight of the observations against the background state.

4. RESULTS

Observations by ACEFTS v3.5 are used to evaluate our analysis. ACEFTS v2.2 (the latest validated version) N_2O is found to agree against independent observations between $\pm 15\%$ between 6-30 km and between ± 4 ppbv between 30-60 km (Strong et al., 2008). For CH_4 , ACEFTS v2.2 is found to agree against independent observations within $\pm 10\%$ in the upper troposphere lower stratosphere, and within $\pm 25\%$ in the middle and higher stratosphere up to the lower mesosphere ($< 60\text{km}$, De Mazière et al., 2008).

In the following, \mathbf{B} and \mathbf{B}_u will denote, respectively, the calibrated and un-calibrated background error covariance matrix.

4.1. Impact of Averaging Kernels and \mathbf{B}

The impact of the use of AK are shown in Figure 4 using N_2O - CH_4 correlations for 2010 in the space of ACEFTS. In addition to ACEFTS data, the correlations from three different BASCOE experiments are shown: an experiment without the use of AK and with \mathbf{B}_u , an experiment with the use of AK and with \mathbf{B}_u and an experiment with the use of AK and the use of \mathbf{B} . The experiment using \mathbf{B}_u assumes 5% of background error standard deviation and Gaussian spatial correlations with 800 km of horizontal length scale and 1 level of vertical length scale. Each correlation plot is fitted to a polynomial and the residual is shown on the plots. The use of AK and/or \mathbf{B} provides N_2O - CH_4 more compact correlations more compact than when it is not the case. From the reduction of the residual of the fit, both the contributions of AK and \mathbf{B} seems to be equivalent in the improvement of the analyses.

Another way to evaluate the impact of AK and \mathbf{B} is to look at the analyses. Figure 5 displays maps of N_2O around 100 hPa (model level 25) on June 15, 2008 from four different BASCOE runs: a model run without assimilation, and the same three runs as in Figure 4. Again, the use of the AK and \mathbf{B} both contribute to improve the N_2O distribution in the Tropics, from a very noisy field to a field much more smooth. N_2O being produced at the Earth surface and having a very long live time (> 100 years), noisy N_2O fields in the Tropics are not expected.

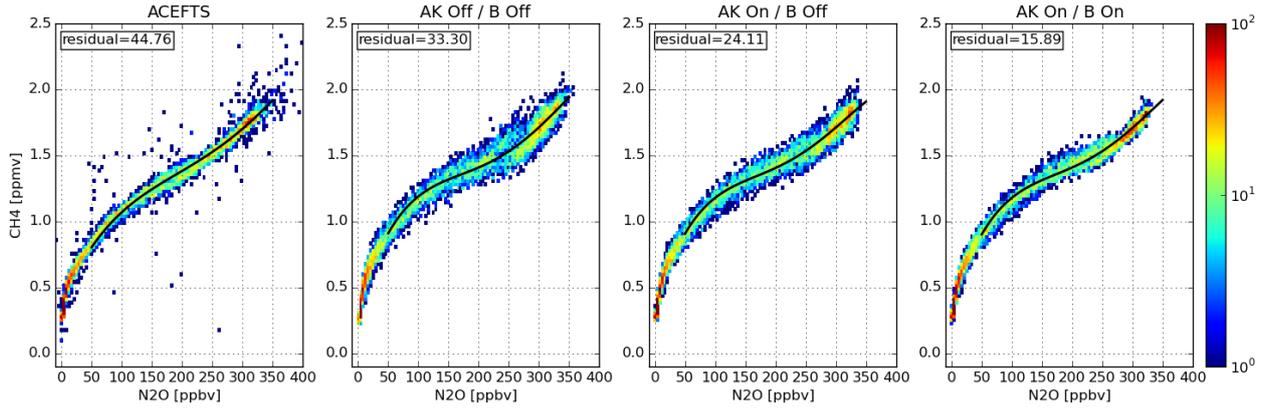


Figure 4. N_2O - CH_4 correlations from ACEFTS, BASCOE without AK and un-calibrated **B**, BASCOE with AK and un-calibrated **B** and BASCOE with AK and calibrated **B** (from left to right). The correlations are for 2010 and between $30^\circ S$ - $30^\circ N$ and BASCOE correlations are shown in the space of ACEFTS.

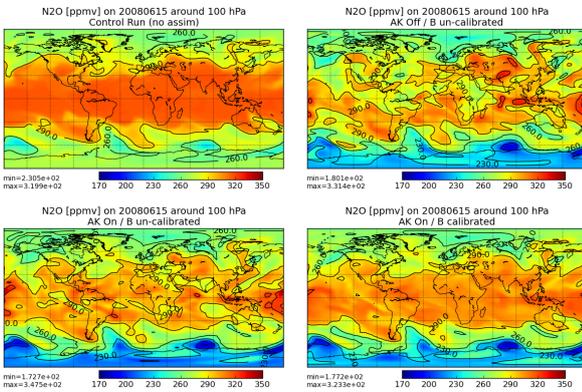


Figure 5. N_2O analysis on June 15, 2008 around 100 hPa (model level 25) from the CTM run, BASCOE without AK and un-calibrated **B**, BASCOE with AK and un-calibrated **B** and BASCOE with AK and calibrated **B** (from top left to bottom right).

4.2. Validation

Figure 6 shows the mean and standard deviation of the difference ACEFTS-BASCOE reanalysis for four season of 2010 in the Tropics and at South Pole, for CH_4 and N_2O . BASCOE CH_4 and ACEFTS agree usually in the range $5\% \pm 8\%$, depending the region and altitude, a good agreement given the value found by De Mazière et al. (2008). For N_2O , the agreement between BASCOE and ACEFTS is in the range $4\% \pm 8\%$, which is also good given the values found by Strong et al. (2008). Usually, the standard deviations are below 5% except during the polar vortex when this value increases to 8% and 10% for CH_4 and N_2O , respectively.

Figure 6 validate the BASCOE analysis in 2010. In order to evaluate the BASCOE reanalysis over the period of MIPAS observations, Figure 7 shows the N_2O time series in the tropics from BASCOE, MIPAS and Aura MLS.

White areas are periods/regions where no data are available. BASCOE reanalysis is available every day. Days without observations are covered by a model simulation. Time series of BASCOE reanalysis displays discontinuities that are also in by MIPAS. These discontinuities do not seem natural, at least they are not observed by MLS (note that MLS also displays discontinuities not observed by MIPAS and at different times). Between mid-2005 and end-2006, many days are not observed by MIPAS and the agreement between BASCOE and MLS is not very good, in particular above 10 hPa. Thus, the validity of the reanalysis may only cover the period January 2007 - April 2012.

Similarly, Figure 8 shows the time series of CH_4 in the tropics from BASCOE reanalysis and MIPAS. Here, the discontinuities appear to be even more pronounced both in observations and analyses. On the other hand, the maximum in MIPAS CH_4 profiles around 20 hPa is removed in BASCOE by the use of the averaging kernels. Nevertheless, these discontinuities make the current version of the reanalysis not valid for CH_4 . Work is in progress to improve the reanalysis. Area of improvements may be by either bias correcting MIPAS observations for days with unrealistic discontinuities or by replacing these analyses by a model simulation. We are also looking forward to the use of MIPAS ESA v7 which will be released in the coming months, hoping for improvements in the stability of the retrieved profiles.

5. CONCLUSIONS

This study presents a reanalysis of MIPAS ESA v6 CH_4 and N_2O made by the Belgian Assimilation System for Chemical Observations (BASCOE). While MIPAS is assimilated between January 2005 - April 2012, the reanalysis is not valid before January 2007 due to the low number of MIPAS observations before that time. The reanalysis agree generally very well with ACEFTS v3.5 obser-

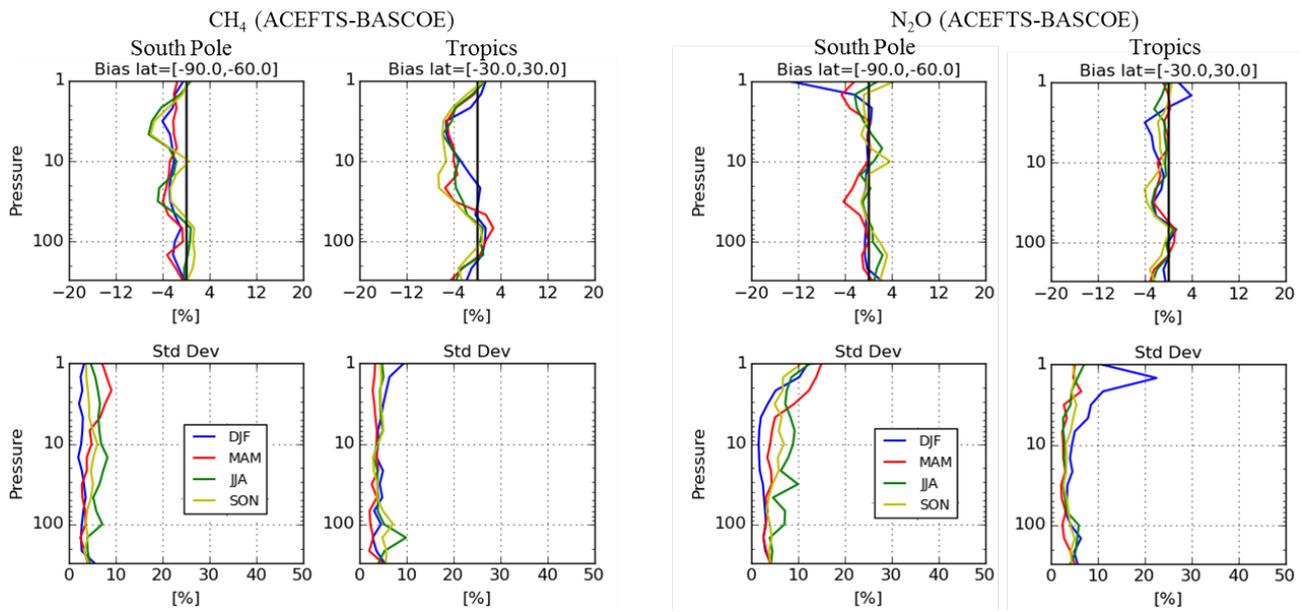


Figure 6. Mean differences (top row) and standard deviation (bottom row) of ACEFTS minus BASCOE reanalysis for each seasons of 2010, for CH_4 and N_2O .

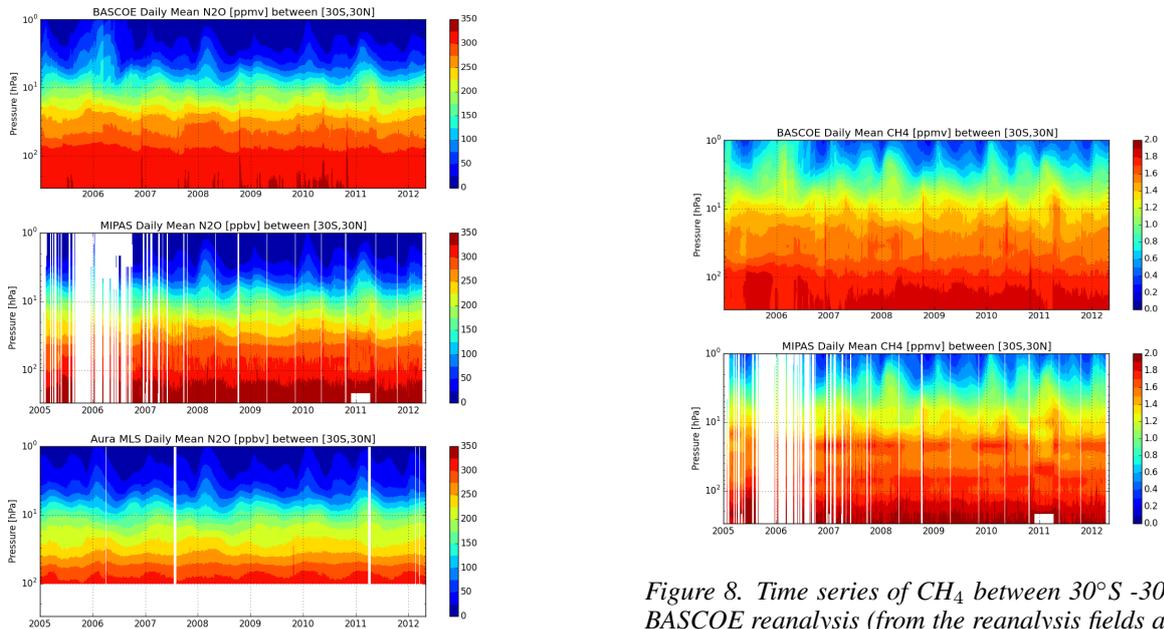


Figure 7. Time series of N_2O between 30°S - 30°N from BASCOE reanalysis (from the reanalysis fields at 12 UT, top), the MIPAS daily mean (middle) and Aura MLS daily mean (bottom).

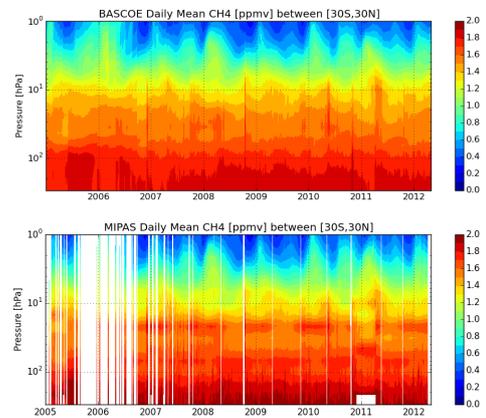


Figure 8. Time series of CH_4 between 30°S - 30°N from BASCOE reanalysis (from the reanalysis fields at 12 UT, top) and the MIPAS daily mean (bottom).

vations in all regions/periods after 2007. Nevertheless, the reanalysis displays discontinuities in time due to the assimilated MIPAS observations such that the reanalysis requires filtering/averaging, in particular in the equatorial lower stratosphere.

The study also shows the added value by data assimilation (DA) method to MIPAS data. DA methods allow one to use more than observations and their errors. Here, the use of the averaging kernels of each profiles greatly improves the representation of the analysis, in particular in the equatorial lower stratosphere, where the MIPAS profiles display unexpected oscillations. Moreover, DA methods also use a priori information which is encapsulated in 4D-Var in the background error covariance matrix (**B**). This study found that calibrating the **B** matrix also improves the analysis, providing much more compact N₂O-CH₄ correlations and in better agreement with ACEFTS.

In the near future, BASCOE will assimilate new ESA retrieval (v7) of MIPAS from where we hope to improve the time stability of the observations and thus the reanalyses. Reanalyses of MIPAS observations of CFC-11, CFC-12 and HCFC-22 (this later being a new product of MIPAS v7) will also be done by BASCOE.

ACKNOWLEDGMENTS

This study was initiated by the study group on the added-value of chemical data assimilation in the stratosphere and upper-troposphere, sponsored by the International Space Science Institute (ISSI).

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